Kittusamy Senthilkumar

List of Publications by Year
in descending order

121	3,070	236612	182168
papers	citations	25 h-index	51 g-index

123	123	123	3372
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Charge Transport Properties in Discotic Liquid Crystals:â€‰ A Quantum-Chemical Insight into Structureâ^'Property Relationships. Journal of the American Chemical Society, 2004, 126, 3271-3279.	6.6	464
2	Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies. Journal of Chemical Physics, 2003, 119, 9809-9817.	1.2	395
3	Absolute Rates of Hole Transfer in DNA. Journal of the American Chemical Society, 2005, 127, 14894-14903.	6.6	325
4	Mapping the Sites for Selective Oxidation of Guanines in DNA. Journal of the American Chemical Society, 2003, 125, 13658-13659.	6.6	97
5	N-heterocycles as corrosion inhibitors for mild steel in acid medium. Journal of Molecular Liquids, 2016, 216, 42-52.	2.3	94
6	Charge Transport in Self-Organized Ï€-Stacks ofp-Phenylene Vinylene Oligomers. Journal of Physical Chemistry B, 2005, 109, 18267-18274.	1.2	90
7	Graphene Quantum Dot Solid Sheets: Strong blue-light-emitting & photocurrent-producing band-gap-opened nanostructures. Scientific Reports, 2017, 7, 10850.	1.6	61
8	Calculation of ionization potential and chemical hardness: A comparative study of different methods. International Journal of Quantum Chemistry, 2009, 109, 764-771.	1.0	59
9	Copper(I) hydrazone complexes: Synthesis, structure, DNA binding, radical scavenging and computational studies. Inorganic Chemistry Communication, 2011, 14, 1318-1322.	1.8	53
10	Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds. Journal of the Royal Society Interface, 2008, 5, 207-216.	1.5	49
11	Quantum chemical studies on tautomerism of barbituric acid in gas phase and in solution. Journal of Computer-Aided Molecular Design, 2002, 16, 263-272.	1.3	47
12	Optical Absorption and Emission Properties of Fluoranthene, Benzo[k]fluoranthene, and Their Derivatives. A DFT Study. Journal of Physical Chemistry A, 2011, 115, 14647-14656.	1.1	41
13	Ultrasonic, DFT and FT-IR studies on hydrogen bonding interactions in aqueous solutions of diethylene glycol. Journal of Molecular Liquids, 2015, 202, 115-124.	2.3	38
14	Structural and Spectral Properties of 4-Bromo-1-naphthyl Chalcones: A Quantum Chemical Study. Journal of Physical Chemistry A, 2011, 115, 6594-6602.	1.1	36
15	Ab initio and DFT studies on structure and stability of aliphatic aldoxime molecules. Computational and Theoretical Chemistry, 2001, 535, 61-70.	1.5	33
16	Coordination Behavior of Acylthiourea Ligands in Their Ru(II)â€“Benzene Complexesâ”€Structures and Anticancer Activity. Organometallics, 2022, 41, 1621-1630.	1.1	33
17	Effect of structural fluctuations on charge carrier mobility in thiophene, thiazole and thiazolothiazole based oligomers. Physical Chemistry Chemical Physics, 2013, 15, 17947.	1.3	32
18	Theoretical and experimental evaluation of a new organic proton transfer crystal aminoguanidinium p-nitrobenzoate monohydrate for optical limiting applications. Journal of Physics and Chemistry of Solids, 2017, 111, 82-94.	1.9	31

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19	Theoretical studies on the quinoidal thiophene based dyes for dye sensitized solar cell and NLO applications. Physical Chemistry Chemical Physics, 2014, 16, 21496-21505.	1.3	30
20	Copper Ion Mediated Selective Cleavage of Câ€“S Bond in Ferrocenylthiosemicarbazone Forming Mixed Geometrical [(PPh₃)Cu(Ï¼-S)₂Cu(PPh₃)₂] Having Cu₂S₂ Core: Toward a New Avenue in Copperâ€“Sulfur Chemistry. Inorganic Chemistry, 2012, 51, 3525-3532.	1.9	29
21	Graphene Nanobuds: A New Second-Generation Phosgene Sensor with Ultralow Detection Limit in Aqueous Solution. ACS Applied Materials & Interfaces, 2019, 11, 19339-19349.	4.0	27
22	Interactions of anticancer drugs with usual and mismatch base pairs â€" Density functional theory studies. Biophysical Chemistry, 2008, 136, 50-58.	1.5	26
23	Mechanism and Kinetics of the Atmospheric Oxidative Degradation of Dimethylphenol Isomers Initiated by OH Radical. Journal of Physical Chemistry A, 2013, 117, 4611-4626.	1.1	26
24	Synthesis and characterization studies of ZnSe quantum dots. Journal of Materials Science: Materials in Electronics, 2012, 23, 2048-2052.	1.1	25
25	Theoretical studies on the reaction mechanism and kinetics of the atmospheric reactions of 1,4-thioxane with OH radical. Structural Chemistry, 2012, 23, 1475-1488.	1.0	25
26	Theoretical investigation of interaction between psoralen and altretamine with stacked DNA base pairs. Materials Science and Engineering C, 2012, 32, 423-431.	3.8	25
27	Theoretical investigation on the structure and antioxidant activity of (+) catechin and (â^') epicatechin â€" a comparative study. Molecular Physics, 2020, 118, e1745917.	0.8	24
28	Two-Dimensional Charge Delocalization in X-Shaped Phenylenevinylene Oligomers. Chemistry of Materials, 2006, 18, 2118-2129.	3.2	23
29	Oxidation and Nitration of Tyrosine by Ozone and Nitrogen Dioxide: Reaction Mechanisms and Biological and Atmospheric Implications. Journal of Physical Chemistry B, 2014, 118, 3479-3490.	1.2	23
30	Structural diversity in aroylthiourea copper complexes â€" formation and biological evaluation of [Cu(<scp>i</scp>)(Ï¼-S)SCl]₂, cis-Cu(<scp>ii</scp>)S₂O₂, trans-Cu(<scp>ii</scp>)S₂O₂and Cu(<scp>i</scp>)S₃cores. New Journal of Chemistry, 2016, 40, 5401-5413.	1.4	23
31	Wurtzite ZnSe quantum dots: synthesis, characterization and PL properties. Journal of Materials Science: Materials in Electronics, 2013, 24, 692-696.	1.1	22
32	Post Hartreeâ€“Fock and density functional theory studies on structure and conformational stability of nitrosoethylene and substituted compounds of nitrosoethylene. Computers & Chemistry, 2002, 26, 207-221.	1.2	20
33	The atmospheric oxidation mechanism and kinetics of 1,3,5-trimethylbenzene initiated by OH radicals â€" a theoretical study. New Journal of Chemistry, 2017, 41, 10259-10271.	1.4	19
34	Origin of the cis effectâ€"nonbonded intramolecular interactions: quantum chemical studies on 1,2-dihaloethylene molecules. Computational and Theoretical Chemistry, 2002, 589-590, 95-102.	1.5	18
35	Tautomerization and solvent effects on the absorption and emission properties of the Schiff baseN,Nâ€²-bis(salicylidene)-p-phenylenediamine â€" A TDDFT study. Molecular Physics, 2010, 108, 1817-1827.	0.8	18
36	Structural, optical, and charge transport properties of cyclopentadithiophene derivatives: a theoretical study. Structural Chemistry, 2014, 25, 715-731.	1.0	18

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37	Absorption and emission properties of phenylene ethynylene oligomers: effect of substitution and Ï€-conjugation length. Molecular Physics, 2009, 107, 1629-1639.	0.8	17
38	Lennardâ^'Jones Parameters for B3LYP/CHARMM27 QM/MM Modeling of Nucleic Acid Bases. Journal of Chemical Theory and Computation, 2009, 5, 396-410.	2.3	17
39	Structure and spectral properties of l-histidinium dipicrate dihydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 102-111.	2.0	17
40	Triazolyl-donorâ€“acceptor chromophore-decorated unnatural amino acids and peptides: FRET events in a Î²-turn conformation. Chemical Communications, 2014, 50, 433-435.	2.2	17
41	Adsorption of RGD tripeptide on anatase (001) surface â€“ A first principle study. Computational Materials Science, 2015, 104, 124-129.	1.4	16
42	Ab Initio QM/MM Modeling of the Rate-Limiting Proton Transfer Step in the Deamination of Tryptamine by Aromatic Amine Dehydrogenase. Journal of Physical Chemistry B, 2017, 121, 9785-9798.	1.2	16
43	Charge Transfer in Polypeptides:â€‰ Effect of Secondary Structures on Charge-Transfer Integral and Site Energies. Journal of Physical Chemistry A, 2006, 110, 11551-11556.	1.1	15
44	Charge transport and optical properties of cross-conjugated organic molecules: A theoretical study. Organic Electronics, 2014, 15, 1607-1623.	1.4	15
45	Effect of Structural Fluctuations on Charge Carrier Dynamics in Triazene Based Octupolar Molecules. Journal of Physical Chemistry C, 2014, 118, 27754-27762.	1.5	14
46	A theoretical study on optical and charge transport properties of anthra-[1,2-b:4,3-bâ€²:5,6-bâ€³:8,7-bâ€´]tetrathiophene molecules. Chemical Physics, 2014, 433, 48-59.	0.9	14
47	Mechanism and Kinetics of the Reaction of Nitrosamines with OH Radical: A Theoretical Study. International Journal of Chemical Kinetics, 2017, 49, 339-353.	1.0	14
48	Mechanism and kinetics of diuron oxidation by hydroxyl radical addition reaction. Environmental Science and Pollution Research, 2020, 27, 12080-12095.	2.7	14
49	Structure, conformation and NMR studies on 1,2-dioxane and halogen substituted 1,2-dioxane molecules. Computational Biology and Chemistry, 2003, 27, 173-183.	1.1	13
50	Structural properties and the effect of platinum drugs with DNA base pairs. Structural Chemistry, 2013, 24, 583-595.	1.0	13
51	Dissociation of N2O on anatase TiO2 (001) surface â€“ The effect of oxygen vacancy and presence of Ag cluster. Applied Surface Science, 2016, 389, 1220-1232.	3.1	13
52	Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical: Hydrogen and Chlorine Atom Abstraction Reactions. Journal of Physical Chemistry A, 2019, 123, 8954-8967.	1.1	13
53	Investigation on surface interaction between graphene nanobuds and cerium(III) via fluorescence excimer, theoretical, real water sample, and bioimaging studies. Materials Chemistry and Physics, 2021, 264, 124453.	2.0	13
54	Hartree-Fock and density functional theory studies on ionization and fragmentation of halomethane molecules by positron impact. Molecular Physics, 2002, 100, 3817-3822.	0.8	12

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55	Effect of substitution of electron-donating and -withdrawing groups on the stability of flavinâ€“diaminepyridine complexesâ€”a density functional theory study. Computational and Theoretical Chemistry, 2006, 758, 107-112.	1.5	12
56	Reaction mechanism of cysteine proteases model compound HSH with diketone inhibitor PhCOCOCH_{3â^’n}X_n, (X = F, Cl,n= 0, 1, 2). International Journal of Quantum Chemistry, 2010, 110, 1660-1674.	1.0	12
57	Atmospheric Oxidation Mechanism and Kinetics of Hydrofluoroethers, CH₃OCF₃, CH₃OCHF₂, and CHF₂OCH₂CF₃, by OH Radical: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 4972-4982.	1.1	12
58	Structural properties and the effect of interaction of alkali (Li+, Na+, K+) and alkaline earth (Be2+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 57-65.	1.1	11
59	Understanding the absorption and emission spectra of borondipyrromethene dye and its substituted analogues. Molecular Physics, 2012, 110, 445-456.	0.8	11
60	Aggregation induced emission behavior in oleylamine acetone system and its application to get improved photocurrent from In2S3 quantum dots. Scientific Reports, 2020, 10, 19712.	1.6	11
61	Insight into the photophysics of strong dual emission (blue & green) producing graphene quantum dot clusters and their application towards selective and sensitive detection of trace level Fe³⁺ and Cr⁶⁺ ions. RSC Advances, 2020, 10, 26613-26630.	1.7	11
62	Hydrogen-bonding studies of amino acid side-chains with DNA base pairs. Molecular Physics, 2011, 109, 1995-2008.	0.8	10
63	Hydrogen bond interactions in hydrated acetylsalicylic acid. Computational and Theoretical Chemistry, 2011, 966, 167-179.	1.1	10
64	A theoretical study of structural and electronic properties of pentacene/Al(1 0 0) interface. Journal of Molecular Graphics and Modelling, 2012, 38, 334-341.	1.3	10
65	Effect of dynamic disorder on charge carrier dynamics in Ph4DP and Ph4DTP molecules. RSC Advances, 2015, 5, 38722-38732.	1.7	10
66	Opto-electronic and interfacial charge transfer properties of azobenzene dyes on anatase TiO 2 (001) surface â€“ The effect of anchoring group. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 346, 372-381.	2.0	10
67	A theoretical investigation on the mechanism and kinetics of the gas-phase reaction of naphthalene with OH radical. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	9
68	Effect of site energy fluctuation on charge transport in disordered organic molecules. Journal of Chemical Physics, 2019, 151, 224301.	1.2	9
69	Structural properties and the effect of 2,6â€diaminoanthraquinone on Gâ€tetrad, nonâ€Gâ€tetrads, and mixed tetradsâ€”A density functional theory study. International Journal of Quantum Chemistry, 2011, 111, 3239-3250.	1.0	8
70	First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes â€“ Ab initio and DFT study. Polyhedron, 2011, 30, 1431-1445.	1.0	8
71	Mechanism and kinetics of the reaction of 1,4-thioxane with O3 in the atmosphere â€“ A theoretical study. Chemical Physics Letters, 2012, 525-526, 153-159.	1.2	8
72	Theoretical and experimental studies on the structure and spectroscopic properties of Ni(II) complexes of the type [Ni(L)(PPh3)] [H2L=5-methyl-N-(2-mercaptophenyl)salicylideneimine and 5-chloro-N-(2-mercaptophenyl)salicylideneimine]. Journal of Molecular Structure, 2013, 1037, 367-375.	1.8	8

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73	Simultaneous Reduction of NOx and Soot Using Early Post Injection. , 0, , .		8
74	Theoretical studies on charge transport and optical properties of tris(N-saclicylideneanilines). RSC Advances, 2014, 4, 25969.	1.7	8
75	Forthâ€“back oscillated charge carrier motion in dynamically disordered hexathienocoronene molecules: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 17729-17738.	1.3	8
76	Adsorption of proline, hydroxyproline and glycine on anatase (001) surface: a first-principle study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
77	Theoretical Investigations on the Mechanism and Kinetics of OH Radical Initiated Reactions of Monochloroacetic Acid. Journal of Physical Chemistry A, 2017, 121, 6028-6035.	1.1	8
78	First principle studies on the atmospheric oxidation of HFC-C1436 initiated by the OH radical. New Journal of Chemistry, 2020, 44, 2070-2082.	1.4	8
79	Charge Transport and Optical Absorption Properties of Dibenzocoronene Tetracarboxdiimide Based Liquid Crystalline Molecules: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 3852-3862.	1.1	8
80	A quantative study of the charge-transfer between conjugated thiophene rings in vibrationally excited states. Physica B: Condensed Matter, 2004, 350, 220-223.	1.3	7
81	Theoretical investigation on intramolecular electron transfer in polypeptides. Chemical Physics Letters, 2007, 440, 302-307.	1.2	7
82	Low temperature method for synthesis of starch-capped ZnSe nanoparticles and its characterization studies. Journal of Applied Physics, 2012, 112, 114331.	1.1	7
83	Depletion of atmospheric ozone by nitrogen dioxide: a bifurcated reaction pathway. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	7
84	Reaction mechanism and kinetics of the degradation of bromoxynil initiated by OH radical. RSC Advances, 2014, 4, 7749.	1.7	7
85	Atmospheric oxidation mechanism of OH-initiated reactions of diethyl ether â€“ the fate of the 1-ethoxy ethoxy radical. RSC Advances, 2016, 6, 81354-81363.	1.7	7
86	Synthesis, structural characterization, DNA/protein binding and inÂvitro cytotoxicity of three structurally different organoruthenium metallates from single pot. Journal of Organometallic Chemistry, 2016, 825-826, 83-99.	0.8	7
87	Unimolecular decomposition of acetyl peroxy radical: a potential source of tropospheric ketene. Physical Chemistry Chemical Physics, 2020, 22, 26819-26827.	1.3	7
88	The influence of the shape and configuration of sensitizer molecules on the efficiency of DSSCs: a theoretical insight. RSC Advances, 2021, 11, 5556-5567.	1.7	7
89	Study of chemical bonding in H2 and HF molecules: Wave function and density functional theory (DFT) parameters approach. International Journal of Quantum Chemistry, 2000, 76, 662-669.	1.0	6
90	Effect of conformational degrees of freedom on the charge transfer in model tripeptide. Journal of Molecular Graphics and Modelling, 2009, 27, 784-791.	1.3	6

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91	Reaction mechanism and kinetics of the atmospheric oxidation of 1,4-thioxane by NO₃Ââ€" A theoretical study. Canadian Journal of Chemistry, 2012, 90, 384-394.	0.6	6
92	Charge transport and optical properties of discotic liquid crystalline molecules THDDP and substituted THDP. International Journal of Quantum Chemistry, 2012, 112, 713-723.	1.0	6
93	A theoretical probe on the non-covalent interactions of sulfadoxine drug with pi-acceptors. Journal of Molecular Structure, 2014, 1074, 157-167.	1.8	6
94	Theoretical probe on modified organic dyes for high-performance dye-sensitised solar cell. Current Applied Physics, 2018, 18, 1071-1079.	1.1	6
95	Studies of chemical hardness and Fukui function using the exact solution of the density functional theory. International Journal of Quantum Chemistry, 2001, 81, 4-10.	1.0	5
96	A theoretical study on decomposition and rearrangement reaction mechanism of trichloroacetyl chloride (CCl₃COCl). International Journal of Quantum Chemistry, 2011, 111, 3482-3496.	1.0	5
97	Opto-electronic properties of low band gap fused-ring thieno[3,4-b]pyrazine analogues â€" A theoretical study. Molecular Physics, 2013, 111, 3036-3046.	0.8	5
98	Theoretical study on the gas phase reaction of methyl chavicol with hydroxyl radical. Computational and Theoretical Chemistry, 2019, 1151, 78-90.	1.1	5
99	Hydrolysis of HNSO₂: A potential route for atmospheric production of H₂SO₄ and NH₃. International Journal of Quantum Chemistry, 2020, 120, e26182.	1.0	5
100	Reaction mechanism and kinetics of the degradation of terbacil initiated by OH radical â€" A theoretical study. Chemical Physics, 2018, 501, 110-120.	0.9	4
101	Mechanism and kinetics of the reaction of methyl acetate with Cl atom â€" A theoretical study. Computational and Theoretical Chemistry, 2018, 1131, 40-50.	1.1	4
102	Room temperature weakly ferromagnetic energy band opened graphene quantum dot coupled solid sheets â€" A possible carbon based dilute magnetic semiconductor. Applied Surface Science, 2021, 548, 149195.	3.1	4
103	Mechanism and kinetics of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical: a theoretical study. Structural Chemistry, 2014, 25, 1773-1783.	1.0	3
104	Adsorption of tetracyanoquinodimethane and tetrathiafulvalene on aluminium (100) surface â€" a first principle study of structural and electronic properties. Molecular Simulation, 2019, 45, 492-500.	0.9	3
105	Mechanism and kinetics of the oxidation of dimethyl carbonate by hydroxyl radical in the atmosphere. Environmental Science and Pollution Research, 2019, 26, 3357-3367.	2.7	3
106	Mechanism, Kinetics, and Ecotoxicity Assessment of Â·OH-Initiated Oxidation Reactions of Sulfoxaflor. Journal of Physical Chemistry A, 2021, 125, 10052-10064.	1.1	3
107	Modified fullerenes as acceptors in bulk heterojunction organic solar cells â€" a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 27468-27476.	1.3	3
108	Post Hartreeâ€"Fock and density functional theory studies on Di-Protonated Allopurinol2+. Computational and Theoretical Chemistry, 2007, 810, 25-30.	1.5	2

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109	Longâ€range charge transfer in donorâ€peptide bridgeâ€acceptor model systemsâ€”A theoretical study. International Journal of Quantum Chemistry, 2011, 111, 3904-3914.	1.0	2
110	Adsorption of perfluoropentacene on aluminum (100) surface: Structural and electronic properties from first principle study. Computational Materials Science, 2014, 89, 216-223.	1.4	2
111	Counter anion effect on structural, opto-electronic and charge transport properties of fused Ï€-conjugated imidazolium compound. Molecular Physics, 2018, 116, 1145-1152.	0.8	2
112	Theoretical Investigation on the Mechanism and Kinetics of Atmospheric Reaction of Methyldichloroacetate with Hydroxyl Radical. Journal of Physical Chemistry A, 2018, 122, 9316-9325.	1.1	2
113	Molecular structure, conformational stability and cis effect of 1,4-dichlorobutadiene â€” a quantum chemical study. Computational and Theoretical Chemistry, 2002, 577, 69-79.	1.5	1
114	Conversion of toluene into benzyl radical on anatase TiO 2 (0 0 1) surface. Computational and Theoretical Chemistry, 2017, 1115, 13-21.	1.1	1
115	Exploring the mechanisms for the radical induced damage of 6â€thioguanine. International Journal of Quantum Chemistry, 2018, 118, e25544.	1.0	1
116	FOBEZ-256 (A hashing function using Bezier curve). , 2010, , .		0
117	Atmospheric oxidation mechanism and kinetics of 2-bromo-4,6-dinitroaniline by OH radicals â€“ a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 21109-21127.	1.3	0
118	A comprehensive quantum chemical study on the mechanism and kinetics of atmospheric reactions of 3-chloro-2-methyl-1-propene with OH radical. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
119	Adsorption of phenanthroline and its derivatives on Au (1Â1Â1) surface â€“ Influence of substitution on structure and electronic properties. Computational Materials Science, 2020, 182, 109778.	1.4	0
120	Crossover from static to dynamic Non-Condon effecton charge Transport in Organic Semiconductors. Journal of Physics: Conference Series, 2021, 1916, 012230.	0.3	0
121	Theoretical studies on adsorption of organic molecules on metal surface. , 2017, , 209-241.		0